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COMPATIBILITY OF RANC-IV ROUTINES WITH AN EXTENDED HEAVE MODEL (U)

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FINAL REPORT

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ABSTRACT

This report documents a study of the interrelationship of RANC IV "heave" model and other phenomenology and effects models in the RANC IV code.

This report is classified CONFIDENTIAL, Group 3, based on the aggragate of the information contained therein.

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SECTION 1

SUMMARY

This report documents a study of the logical connections between various RANC-IV phenomenology and effects models and the RANC-IV "heave" model. The purpose of the study was to delineate routines or models which:

(a) were implicitly or explicitly dependent on the present structure of the "heave" model and, hence, would require modification or reformulation with a new or extended "heave" model;

(b) had information requirements which would affect the design of any extended "heave" model.

The extended "heave" model under primary consideration was a coarse grained three-dimensional forward-in-time hydromagnetic computation.

As one might expect, the principal interaction of the RANC-IV code and the "heave" model is in the computation of E-F region ionization. This is also the computational area which most seriously affects the structure of an extended "heave" model. So long as the current modeling approach in which "fireballs" are geometric regions superimposed on the "heave" flow field is maintained, all of the intersection routines, for example, can be carried over intact. The already-present logical division between altitude points above and below 100 km enables all the computations below 100 km to be continued as is, independent of the models above 100 km.

The phenomenology models are almost entirely dependent on the burst point mass density rather than any other specific properties and hence are almost immediately compatible with any "heave" model in which interpolation for total mass density at an arbitrary point is included. There are several instances where the atmospheric scale-height is used but this dependence should be easily eliminated. The dependence, in several instances, on atmospheric density at the current fireball/debris location can also be accommodated with a density interpolation routine.

Perhaps the most serious complication in the phenomenology package arises through the RMASS subroutine which is used to (a) compute the "equal mass" (per steradian) distance in the vertically down or up directions from the burst point or (b) compute the mass per steradian to a given distance. Currently the routine uses the atmospheric density and scale height at various points along the integration path. This routine will require restructuring to be compatible with the information available from the "heave" model. The form of the modification depends on the form of the "heave" model.

The most useful and timely procedure for upgrading the "heave" computations to the current state-of-the-art in multidimensional MHD calculations appears to be the use of such a code or codes as a "driver" package providing precomputed flow field and ionizing flux information, throughout a three-dimensional mesh. With minor and/or trivial modifications, the remainder of the code is compatible with such a data bank replacing the ATMOSF and PIONF routines.

SECTION 2

INTRODUCTION

The RANC IV "heave" model, that is, the calculation of the Eulerian trajectory and relative volume for an air parcel is actually a subprogram of the ATMOSF routine and need not be considered separately. This latter routine provides for a given point in space and time basically the following information, depending on the chosen "mode" control.

MODE 1

Z_j - altitude array for this air parcel

ρ_j - density array for this air parcel

H_{s_j} - scale height array for this air parcel

t_j - time array for this air parcel (burst times plus required intermediate time)

v - vertical velocity at current time

$[N_2]_0$ - initial molecular nitrogen concentration in this air parcel

$[O_2]_0$ - initial molecular oxygen concentration in this air parcel

$[O]_0$ - initial atomic oxygen concentration in this air parcel

T - temperature at initial altitude

M - mean molecular weight at initial altitude

MODE 0

Z	-	altitude at the current time
ρ	-	density at the current time
H_S	-	density scale-height at the current time
v	-	vertical velocity at the current time
T	-	temperature at current time (γ-law expansion from initial time)
$[N_2]$	-	N_2 concentration at current time } no chemistry, i.e., volume expansion only
$[O_2]$	-	O_2 concentration at current time
[O]	-	O concentration at current time
M	-	mean molecular weight at initial altitude

Mode 1 provides the same type of information for Mode 0 with the additional constraint that the air parcel is in the same vertical column and the time of interest is the same as for the immediately preceding call of the ATMOSF routine. This is a simplification which in the case of a "heaved" atmosphere does not require recalculation of x-ray energy deposition in the air column. From the viewpoint of replacing the current "heave" model this mode need not be considered separately from Mode 0. Of particular relevance to this study, the RANC-IV "heave" model treats multiburst heave as a superposition of single burst effects and hence the time required to calculate a "heave" trajectory increases linearly with the number of bursts.

Clearly, the simplest, although not the most efficient or useful, procedure for replacing the RANC IV "heave" model is to simply take the listed outputs above as the output specification for any other "heave" model. The remaining portions of the code are then completely compatible. More usefully, the routines which make use of this information should be examined and alternate formulations or sources for the information considered. This is accomplished in the following sections.

SECTION 3

RMASS SUBROUTINE

This routine calculates the atmospheric mass per steradian to a given radius in a vertically up or down direction from the burst point. (Alternately, the routine calculates the radius to a given mass per steradian.) The integration algorithm assumes an exponential variation in density over one-half the local scale height. Because the integration is along a vertical column all ATMOSI calls use Mode-1.

This routine is used only by the fireball/debris phenomenology (PHENOM) routine to establish "initial" vertical dimensions and the upward expansion velocity. Within the context of a three-dimensional atmospheric model the current integration scheme is probably not justified since density information would proably only be available on, say, a one scale-height vertical grid.

This routine will require modification, assuming the phenomenology package is unchanged (in the sense of "initial" fireball sizing). The form of the modification depends on the form of the atmospheric density model. Three approaches to this problem have been proposed.

(a) If the E-F Region atmospheric model is a three-dimensional hydrodynamic code, the modification is quite straightforward. Such an atmospheric model will require a procedure for depositing radiated energy within the mesh and whatever procedure is used can be directly applied to the "fireball" (e.g., single ionization and dissociation) dimensions.

(b) If the chosen atmospheric model is a "fit" to more detailed two- or three-dimensional calcualtions then the mass integrals need to be formulated in terms of the available parameters (perhaps a power-law exponent or exponential scale height).

(c) If the atmospheric model is a tabular one, based on more detailed calculations, the integration algorithm required is the same as for option (a) (assuming a procedure for interpolation in yield, burst altitude and burst timing can be constructed).

SECTION 4

PHENOM SUBROUTINE

The fireball/debris scaling routine (PHENOM) uses ATMOSF for several purposes:

(a) burst point density and scale height

(b) fireball "bottom" density, scale height, and "heave" velocity

(c) altitude at which $\rho = 3.3 \times 10^{-15}$ g/cm^3

(d) density and scale height at current debris center location

(e) altitude at which $\rho = 1.6 \times 10^{-13}$ g/cm^3

Item (a), the burst point density and scale height, is involved in almost all the basic phenomenology scaling relations. Actually, most of the scaling relations make use of only the burst point density, and this represents no real burden on any heave model, requiring only a simple interpolation scheme. The burst point scale height is used for two calculations:

(1) The "uniform density" radius. In estimating the initial position of the upward-moving debris expansion for burst above 120-km altitude, the expansion is assumed to proceed as in a uniform atmosphere, i.e., $R_s \propto t^{2/5}$ until R_s is equal to one-half the density scale-height at the burst point or equal to the horizontal shock radius (at the UV radiation time), whichever is least. Beyond this "switch" radius an empirical radius-time behavior is assumed.

(2) The "containing" mass. Where required, e.g., in the calculation of the terminal expansion velocity upward, the total mass per steradian directly above the burst point is assumed to be $2\rho_B H_{sB}$ where H_{sB} is the burst point scale height. (For a simple exponential atmosphere, this is the correct expression.)

Since the calculation of the upward dimensions is accomplished after those for the horizontal and downward dimensions, the use of the scale-height in item (1) above can be eliminated by using $\sqrt{R_D R_H}$, the geometrical mean radius, instead of one-half the local scale-height, as the "switch" radius.

The other use of the burst point scale-height, i.e., item (2) above, can be removed, although the actual replacement is probably dependent on the form of the "heave" model. If the "heave" model is a coarsely zoned three dimensional MHD computation, then the mass per steradian computation could be performed in a straightforward integration vertically through the mesh.

If the "heave" model is either a tabular model of 3-D computations or an analytic model, the parameters of the respective model will determine the mass integration scheme. Thus, if the analytic density model contains, say, a power-law exponent for altitude variation then a corresponding integration algorithm would be used. Similarly, a tabular model can be "fit" by either a power law or exponential variation between entries and a corresponding algorithm employed.

In summary, item (a) uses of the ATMOSF routine (which are the most numerous) imply very little restriction on the form of the "heave" model requiring essentially an interpolation routine for the atmospheric density at a point.

The second use of the ATMOSF routine by PHENOM, item (b) above, is the determination of the initial density and scale-height at the

"bottom" of the fireball in addition to the "heave" flow field velocity. This former information is used to establish the "total" fireball mass and initial mass density scale-height. Assuming the "heave" model can be processed to yield the "bottom" density, this density, together with the burst point density, can be used to obtain an appropriate scale height. The "heave" model can also be expected to yield the appropriate vertical flow velocity.

The third listed use of ATMOSF, item (c) above, is involved in determining the altitude for charge exchange energy loss for the downward expansion. Since it involves only the density, a fairly simple interpolation scheme within the "heave" model could provide the desired altitude information and this would avoid the necessity for recoding this aspect of the phenomenology model.

Item (d), the density and scale height at the debris altitude, is used in the beta-ray deposition calculation (actually only the pressure at the debris altitude is used for deposition above 120-km altitude). These quantities are used only to modify the penetrated mass from infinity for that fraction above the debris altitude. For high altitude debris sources this correction is never very significant if indeed the ionization is significant. A simple solution for item (d) appears to be to use the corresponding quantities from the "unheaved," e.g. CIRA-65, atmosphere.

Item (e), the final use of the ATMOSF routine by PHENOM, occurs in an attempt to locate the lower edge of a late-time, high-altitude fireball. This density criterion is highly uncertain and could probably be replaced. It can be retained, however, by a density interpolation scheme as discussed above.

SECTION 5

SUBROUTINE PIONF

This subroutine computes the ionization and energy deposition within a given air parcel due to x-ray and UV radiation from a given burst. The routine is used by subroutines ABSORB and ENEF for each burst prior to the time of interest. Subroutine ATMOSF (and hence HEAVE) is used to determine the mass density at several selected points along a ray passing from the burst point to the field point, so that required mass line integrals or specie line integrals can be computed. This is accomplished with a MODE 0 call of ATMOSF. (Note that the relative neutral composition will be that appropriate to undisturbed air originating at the same point as the air in question.) Since for each burst after the first, several,intermediate density calculations are required, say three, each of which involves "heave" due to all burst prior to the one in question, the PIONF routine is actually the source of the N^2 (where N is the number of bursts) dependence of RANC IV computation time. This is demonstrated by considering Figure 1 which illustrates the computation procedure for three bursts. In order to compute the density at three intermediate points for each of the second and third bursts, a total of nine "heave" calculations (and 18 energy deposition calculations) are required. In general,

$$\frac{3}{2}\left(N_{PB}^{2} - N_{PB}\right)$$

"heave" calculations are required, where N_{PB} is the number of bursts prior to the time of interest.

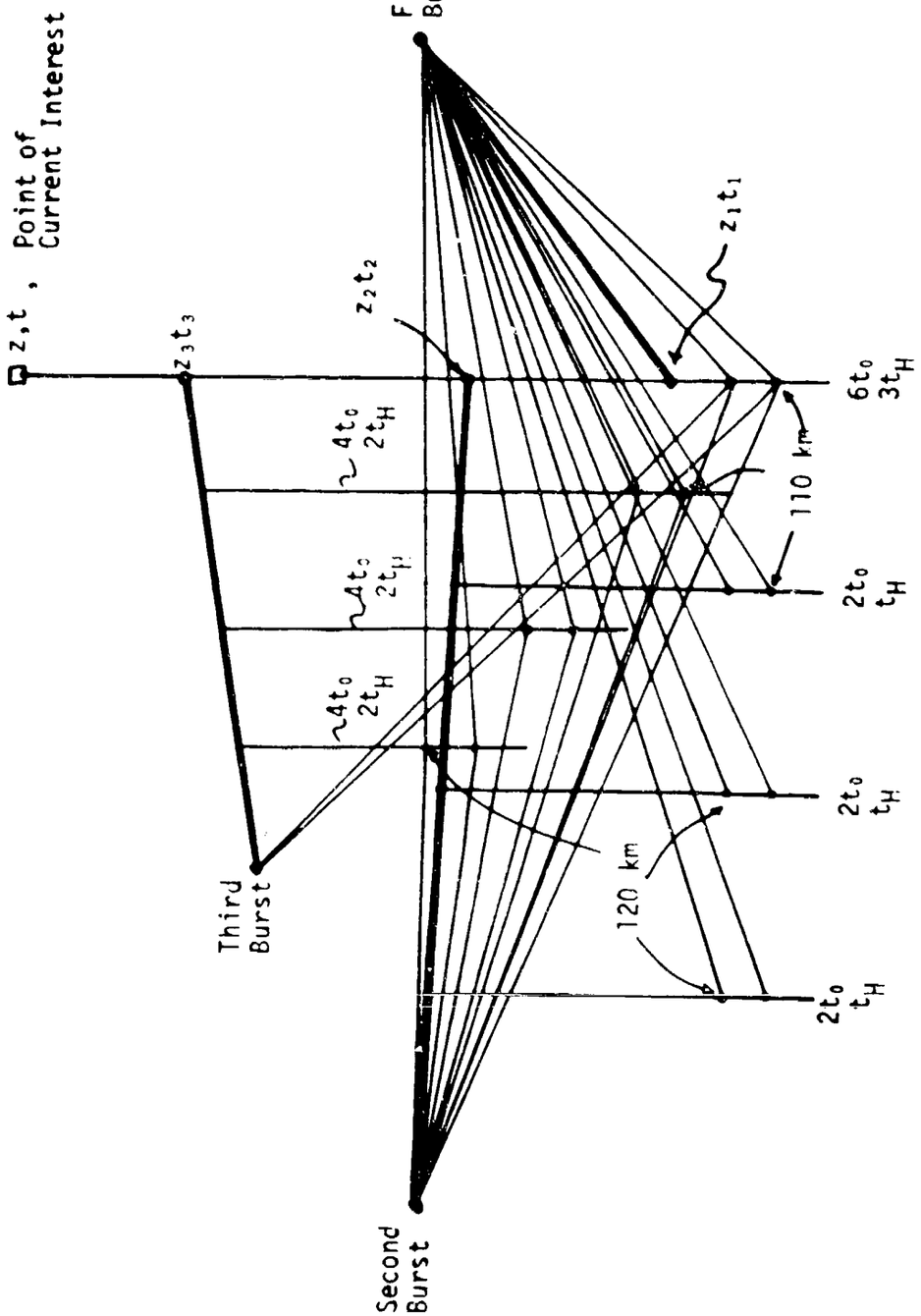

Figure 1. Illustration of Energy Deposition and Heave Calculations Required by ENEF and PIONF Routines for Each Point z,t (Three Preceding Bursts).

It seems almost ironic that the calculation of ionization within the volume element (which is equivalent to computing the x-ray flux and effective absorption coefficient and the three group UV flux at the point in question) although admittedly crude (i.e., no burnout or buildup of species) effectively controls the code running time.

In the context of an extended "heave" model, PIONF can be replaced by any procedure which provides the required x-ray and UV fluxes from each burst at an arbitrary point.* If the "heave" model is a multidimensional MHD code with the ionization chemistry coupled directly to the flow then, of course, the computations currently performed by PIONF are inherent in the "heave" model and need not be separately considered. Such a "heave" computation may not really be feasible in terms of required storage, etc., especially in view of the artificial diffusion of chemical species which occurs in Eulerian codes.

If the "coupled chemistry" approach is not feasible, then an uncoupled approach similar to that of the ZIFF code** is probably preferred. For such an approach, stored tabulations of x-ray and UV fluxes throughout the computational mesh following each burst will be required and this tabulation replaces the PIONF routine. Note that the size of this tabulation increases only as the number of prior bursts, not as N^2 so that an extended heave model, based on a multidimensional MHD computation automatically removes one of the most troublesome aspects of the present code.

*In RANC IV, PIONF actually transforms the fluxes to ion density-produced, but this simple transformation could just as well be performed in the calling routine.

**F. E. Fajen and D. S. Sappenfield, "Numerical Simulation of a High Altitude Nuclear Event," LA-4318-MS, 1/15/70 (S/RD).

SECTION 6

SUBROUTINE ENEF

This routine calculates the electron and ion density history within a Lagrangian air parcel which is located on the ray path of interest at the current time. Subroutine ATMOSF is used to obtain the density history of the volume element of interest and subroutine PIONF (which also uses ATMOSF) is used to obtain the ionization produced by each preceding burst. The ENEF routine is thus primarily a deionization chemistry routine. The charged particle chemistry model is analytic and treats two positive ions (one molecular, one atomic) and electrons. Volume expansion and neutral specie changes are introduced incrementally.

In the context of an extended "heave" model, two possible approaches to this routine can be considered.

(1) If the "heave" model is a multidimensional MHD computation with coupled chemistry, the ENEF routine could be replaced by a simple interpolation scheme to obtain the electron and ion densities at the point in question.

(2) If the "heave" model does not include the required chemistry, then the simplest procedure is to leave the ENEF routine essentially intact.

The first approach while logically simpler requires additional storage and additional computing time for the basic "heave" calculation and yields only coarse grained electron densities. In addition, the computed charged particle densities are subject to the bothersome artificial diffusion characteristic of Eulerian computations. The second

procedure is easier to implement in terms of current computing capability and removes the chemistry model from the details of the "heave" computation, providing in principle, a more finely zoned charged particle distribution not subject to artificial diffusion. In the context of this latter approach, the ENEF routine requires for compatibility:

(a) the initial location and relative density history for the air parcel of interest;

(b) the ionizing radiation fluxes at the volume element following each burst. (The ENEF routine currently obtains the additional ion concentrations directly but this is a trivial change if the fluxes (in each energy group) are available.)

The initial location and density history can be obtained from (a) the initial Lagrangian coordinates corresponding to each Eulerian cell center (as in ZIFF for example); (b) a series of multidimensional flow "dumps" covering preceding burst times and other intermediate times. The ionizing fluxes are probably most appropriately prepared as an additional series of "dumps" during the multidimensional MHD computations.

SECTION 7

SUBROUTINE ABSORB

This subroutine, which calculates path absorption and refraction, chooses a logical set of points at which ionization calculations are required. In determining this set of required points this routine uses subroutine PIONF (which in turn uses ATMOSF) to determine the importance of x-ray and UV ionization from each preceding burst on the ray path of interest by computing the resulting ionization at one point on the path.

Again, two options relative to this routine are possible: (a) the single point calculation is eliminated, possibly leading to inclusion of "unimportant" bursts; (In the context of multidimensional MHD computations with chemistry "all" bursts are automatically included at each point.) (b) the single point calculation is modified to use the ionizing flux "dumps" discussed in the preceding section.

The latter approach is probably more realistic for the short term and requires only trivial modification of ABSORB.

SECTION 8

SUBROUTINE ENEFB

This routine computes electron densities within those regions designated as "fireballs" in EANC-IV. The routine makes three independent calculations of electron density and chooses the largest

(a) thermal equilibrium n_e at current fireball density ρ ;

(b) non-equilibrium n_e following decay from initial single ionization;

(c) beta-ray induced n_e at current fireball density.

In order to calculate by option (a) or (c), mass density at the point within the fireball is required. Since as the burst altitude increases from near sea level to altitudes above, say 100 km, the fireball mass density is alternately determined by (1) entrainment at pressure equilibrium with the surroundings and (2) by the expansion of the initial fireball mass, the density required is taken as the maximum of that corresponding to (1) or (2) above. To determine the pressure equilibrium density the "outside" density and temperature are required and for "fireballs" above 120 km the use of the ATMOSF routine is required. For fireballs at these altitudes this is almost certainly a gratuitous calculation and the use of ATMOSF (and hence "heave") could be easily removed by taking densities and temperatures from the standard (pre-burst) atmosphere.

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